

# CODING FORMS FOR SRC INDEXING

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Submitting Organization	ATOCHEM NORTH AMERICA INC		
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Document Title	INITIAL SUBMISSION: LETTER FROM ATOCHEM NORTH AMERICA INC TO USEPA REGARDING TOXICITY STUDIES OF N-DECYLMERCAPTAN AND N-DOCECYLMERCAPTAN WITH COVER LETTER DATED 07/20/92		
Chemical Category	N-DECYLMERCAPTAN, N-DOCECYLMERCAPTAN		

8(e)

# CAP

(COMPLIANCE AUDIT PROGRAM)

## TSCA CONFIDENTIAL BUSINESS INFORMATION

ORIGINAL - DCO (Jeff/Eric)  
COPY # 1 - CBIC  
COPY # 2 - Scott Sherlock

10406

## COMPANY SANITIZED

ORIGINAL - PINS  
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## CONTAINS NO CBI

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8EHQ - 0892-10406

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July 20, 1992

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8EHQ-92-10406  
INIT 08/04/92

Attn: Section 8(e) Coordinator (CAP Agreement)

RE: Report Submitted Pursuant to the TSCA Section 8(e)  
Compliance Audit Program

CAP Identification Number: 8ECAP-0026

Dear Sir/Madam:

Pursuant to the Toxic Substances Control Act (TSCA) Section 8(e) Compliance Audit Program and the Agreement for TSCA Section 8(e) Compliance Audit Program (CAP Agreement) executed by Elf Atochem North America Inc. (Atochem) and Environmental Protection Agency (EPA), Atochem is submitting the enclosed final report on studies to establish eye irritation potential for n-decylmercaptan and n-dodecylmercaptan in rabbits to the EPA. These studies do not involve effects in humans.

Nothing in this letter or the enclosed studies are considered confidential business information of Atochem.

The enclosed studies provide information on the chemicals n-decylmercaptan and n-dodecylmercaptan. The exact chemical name of n-decylmercaptan is 1-decanethiol and its CAS number is 143-10-2. The exact chemical name of n-dodecylmercaptan is 1-dodecanethiol and its CAS number is 112-55-0.

The title of the enclosed report is Alkyl Mercaptans: Vapor Toxicity and Irritant Properties. This report consists of several studies. The following is a summary of the adverse effects observed in the eye irritation studies with n-decylmercaptan and n-dodecylmercaptan.

TSCA CAP  
N-Dodecylmercaptan and N-Decylmercaptan  
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Page Two

Application of n-decylmercaptan and n-dodecylmercaptan into the eyes of three rabbits was corrosive to the rabbit eye.

To our knowledge, Atochem has not previously submitted any TSCA Section 8(e) notices or premanufacture notifications on the subject chemicals.

Further questions regarding this submission may be directed to me at 215 337-6892.

Sincerely,



C.H. Farr, PhD, DABT  
Manager, Product Safety  
and Toxicology

Enclosures

LABORATORY REPORT *211* *BE* *discussed* *TRM 79-769* *S-782*

CONFIDENTIAL FOR: PENNSALT CHEMICALS CORPORATION  
ATTENTION: DR. JOHN L. EATON

RE: ALKYL MERCAPTANS; VAPOR TOXICITY AND IRRITANT PROPERTIES.

A HOMOLOGOUS SERIES OF SIX ALKYL MERCAPTANS HAVE BEEN INVESTIGATED IN REFERENCE TO (1) VAPOR-TOXICITY IN MICE, (2) PRIMARY SKIN-IRRITATION PROPERTIES WITH RABBITS AND (3) EYE-IRRITATION PROPERTIES WITH RABBITS. THE SERIES OF COMPOUNDS CONSISTED OF THE FOLLOWING:

22	N-PROPYL	MERCAPTAN	2231
20	N-BUTYL	MERCAPTAN	2229
2833	N-AMYL	MERCAPTAN	EC 2662
17	N-OCTYL	MERCAPTAN	2236
2852	N-DECYL	MERCAPTAN	EC 1444
<del>2852</del>	<del>N-DODECYL</del>	<del>MERCAPTAN</del>	<del>2234</del>

COMPLETE DATA OBTAINED IN EACH EXPERIMENT ARE SET FORTH IN THE APPENDED STANDARD LABORATORY FORMS; THE PRESENT REPORT WILL DETAIL THE METHODS USED AND WILL SUMMARIZE AS WELL AS ATTEMPT A COMPARATIVE INTEGRATION OF THE FINDINGS.

METHODS

VAPOR TOXICITY.

VARIOUS ATMOSPHERIC CONCENTRATIONS OF EACH PRODUCT WERE PREPARED IN HERMETICALLY SEALED CHAMBERS OF TWENTY-LITER CAPACITY; SATURATED CONCENTRATIONS OF THE HIGHER HOMOLOGS WERE ACHIEVED BY PLACING ONE-GRAM QUANTITIES WITHIN THE SEALED CHAMBER AND ALLOWING TWENTY-FOUR HOURS FOR EQUILIBRATION AT ROOM TEMPERATURE PRIOR TO USE. NORMAL, HEALTHY, MALE MICE OF THE CF<sub>1</sub> STRAIN SERVED AS THE EXPERIMENTAL ANIMAL. FIVE MICE WERE EXPOSED SIMULTANEOUSLY IN EACH VAPOR CHAMBER FOR A PERIOD OF ONE-HOUR DURING WHICH TIME THEY WERE UNDER CONTINUOUS OBSERVATION FOR THE DEVELOPMENT OF TOXIC EFFECTS; SURVIVORS WERE KEPT FOR AT LEAST FIVE DAYS TO NOTE THE APPEARANCE OF RESIDUAL REACTIONS OR LATE DEATHS AS WELL AS TO ASSURE COMPLETE RECOVERY AS REFLECTED BY NORMAL BODY-WEIGHT-GAIN. THE CONCENTRATIONS USED WERE LOGARITHMICALLY (INCREASING INCREMENTS OF APPROXIMATELY 50%) SPACED AND ENBRACED THE ENTIRE NON-TOXIC TOXIC RANGE TO PERMIT CALCULATION OF THE MEDIAN-LETHAL-CONCENTRATION (LC<sub>50</sub>).

PRIMARY SKIN IRRITATIONS

USING RABBITS AS THE EXPERIMENTAL ANIMAL, EACH PRODUCT WAS APPLIED TO THREE INTACT SKIN AREAS AND TO THREE ABRADED SKIN AREAS FOR A PERIOD OF TWENTY-FOUR HOURS. THIS WAS ACCOMPLISHED BY PLACING 0.5 CC VOLUMES OF THE PRODUCT UPON A GAUZE PAD WHICH WAS THEN SECURED TO THE EXPERIMENTAL SITE WITH ADHESIVE TAPE AND FURTHER SECURED BY AN OVER-LYING RUBBER GIRDLE. AT THE CONCLUSION OF THE TWENTY-FOUR HOUR EXPOSURE PERIOD, THE PATCH WAS REMOVED AND THE SKIN INSPECTED FOR SIGNS OF IRRITATION; SUCH OBSERVATIONS WERE CONTINUED FOR THREE DAYS AND WERE SCORED BY THE METHOD OF GRAZE, ET AL.

N-Decyl Mercaptan CAS # 143-10-2  
N-Dodecyl Mercaptan CAS # 112-55-0



### CORNEAL IRRITATION.

EACH PRODUCT WAS INSTILLED INTO THE EYES OF THREE RABBITS FOR A CONTACT PERIOD OF SIXTY SECONDS AT WHICH TIME THE SURPLUS WAS REMOVED WITH A COTTON SWAB. IN ADDITION, EACH PRODUCT WAS INSTILLED INTO ONE RABBIT EYE FOR A PERIOD OF TEN SECONDS WHEN THE EXCESS WAS FLUSHED AWAY WITH SALINE. THE TREATED EYES WERE THEN EXAMINED PERIODICALLY AND THE DEGREES OF IRRITATION WERE SCORED BY THE METHOD ESTABLISHED BY DRAIZE, ET AL.

### RESULTS

A PROGRESSIVE INCREASE IN VAPOR-TOXICITY WAS OBSERVED WITH THE FIRST THREE MEMBERS OF THE HOMOLOGOUS SERIES OF COMPOUNDS WITH  $LC_{50}$  VALUES AS FOLLOWS:

PROPYL, 17,660 PPM  
BUTYL, 16,670 PPM  
AMYL, 9,040 PPM.

THESE COMPOUNDS SHOWED DISTINCT SIMILARITIES IN THE NATURE OF THE SYMPTOMS PRODUCED AND EACH CAUSED DAMAGE TO THE CENTRAL NERVOUS SYSTEM AS SHOWN BY THE PRESENCE OF RESIDUAL EFFECTS AMONG SURVIVING ANIMALS. THE NEXT MEMBER OF THE SERIES, N-OCTYL MERCAPTAN, CAUSED THE DEVELOPMENT OF TOXIC-SYMPTOMS DURING EXPOSURE TO SATURATED CONCENTRATIONS BUT NO MORTALITIES OCCURRED; RESIDUAL EFFECTS DID NOT APPEAR. THE DECYL AND DODECYL COMPOUNDS WERE COMPLETELY INERT AT SATURATED ATMOSPHERIC CONCENTRATIONS BY GROSS OBSERVATION.

IN REFERENCE TO THE PRIMARY IRRITATION STUDIES, NONE OF THE COMPOUNDS PRODUCED SIGNS OF IRRITATION WHEN APPLIED TO EITHER INTACT-SKIN OR TO ABRADED-SKIN FOR A CONTACT PERIOD OF TWENTY-FOUR HOURS.

WHEN INSTILLED IN THE RABBIT-EYE, EACH PRODUCT OF THE SERIES PRODUCED MARKED IRRITATION WITH THE PROPYL HOMOLOG BEING THE LEAST IRRITATING (COMPLETE RECOVERY WITHIN TWO DAYS) AND THE DECYL AND DODECYL HOMOLOGS BEING THE MOST IRRITATING (NO SIGNS OF RECOVERY WITHIN SEVEN DAYS); WITH THE LATTER TWO COMPOUNDS, STRUCTURAL DAMAGE OF THE IRIS BECAME MANIFEST SEVERAL DAYS FOLLOWING INSTILLATION AND IT WAS THIS EFFECT WHICH INDICATED PROBABLE PERMANENT INJURY. CURIOUSLY, HAIR-LOSS OCCURRED AROUND THE EYES OF THE RABBITS TREATED WITH THE OCTYL, DECYL AND DODECYL HOMOLOGS ONLY.

### SUMMARY

THE DATA OBTAINED IS SUMMARIZED AS FOLLOWS:

N-PH-AEROCAPTAN	LC <sub>50</sub> VAPOR TOXICITY		REMARKS	SKIN IRRITATION		EYE IRRITATION	
	MG/L	PPM		INTACT	ABRADED	MAX. SCORE*	DURATION
PROPYL	60	17,660	CNS DAMAGE	0	0	13	2 DAYS
BUTYL	67	16,670	CNS DAMAGE	0	0	20	4 DAYS
AMYL	42	9,040	CNS DAMAGE	0	0	17	3 DAYS
OCTYL	>SAT.	---	TOXIC SYMPTOMS	0**	-	15+HR	4 DAYS
DECYL	>SAT.	---	---	0	0	26+HR	>7 DAYS
DODECYL	>SAT.	---	---	0	0	25+HR	>7 DAYS

\* MAX. POSSIBLE SCORE = 30; HR = HAIR-LESS PALPEBRAL AREA.

\*\* REPORTED UNDER DATE OF 3/21/57.

IT WOULD APPEAR THAT IRRITANT PROPERTIES AND VAPOR-TOXICITY INCREASE WITH INCREASED LENGTH OF THE ALKYL CHAIN; HOWEVER, THE OCTYL, DECYL, AND DODECYL MEMBERS OF THE PRESENT HOMOLOGOUS SERIES WERE FOUND TO BE NON-TOXIC BY INHALATION PRESUMABLY BECAUSE OF THEIR LOW VOLATILITY.

PHARMACOLOGY RESEARCH, INC.  
MAY 26, 1958

*NK*

## CERTIFICATE OF AUTHENTICITY

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